Anil Kumar

Curriculum Vitae

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Los Alamos National Laboratory
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Employment

Aug, 2013 –Present	**Postdoctoral Research Associate**, Los Alamos National Laboratory, Los Alamos, NM, USA
Supervisor	Jian Wang and Carlos Tome
Concentration	Atomistic simulations and multiscale modeling of hexagonal metals
Sept, 2010 –Aug 2013	**Postdoctoral Research Associate**, Department of Physics and Astronomy, Rutgers University, NJ, USA
Supervisor	Karin Rabe
Concentration	First-principles modeling of complex oxides

Education

2005–2010	**Ph.D.**, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India
Courses	Physics, Materials Science
Supervisor	Umesh V. Waghmare
Concentration	Ferroelectrics, Spin-Phonon Coupling, Superconductivity and Magnetism
2003–2005	**M.Sc.**, Banaras Hindu University, Varanasi, India
Course	Physics
Concentration	Nanomaterials, Effect of Quantum Confinement on the Optical Properties of Semiconductors
2000–2003	**B.Sc.**, Gorakhpur University, Gorakhpur, India
Courses	Physics, Mathematics, Computer Science

Doctoral Thesis

Title	**Phonon Anomalies and Related Phenomena in the Ferroelectrics, Fe-pnictide Superconductors and Spinels**
Supervisor	Umesh V. Waghmare

Master Thesis

Title	**Synthesis and Characterizations of CdSe/CdS Nano-particles**
Supervisors	Anchal Srivastava and O. N. Srivastava

Research Experience

Computational

2010–Present **Postdoctoral Research**

[1] Developed a very simple and efficient scheme to construct first-principles effective Hamiltonian for ferroelectrics using interatomic force constants, which can be used to study structural phase transitions in the system as a function of temperature using classical molecular dynamics or Monte Carlo simulations.

[2] Studied spin-phonon coupling and structural phase transition in cubic spinel structure of $CdCr_2O_7$.

[3] Using first-principles calculations I tried to understand the role of different atomic distortions, magnetic orderings and epitaxial strain to tune metal to insulator transition in highly correlated compounds such as $SrVO_3$, $CaVO_3$, $LaVO_3$ and YVO_3 in the bulk as well as in superlattices.

[4] Worked to understand metal-insulator transition in Ruddlesden-Popper series of $Sr_{n+1}Co_nO_{3n+1}$ using different magnetic orderings and epitaxial strain.

2005–2010 **Ph.D. Student, JNCASR, Bangalore**

[1] Designing and predicting the properties of new materials such as ferroelectrics, multiferroics and superconductivity using first-principles based calculations.

[2] Worked to understand microscopic mechanism behind the cooperative phenomena in materials that leads to the different phase transitions and interesting physical properties

[3] Developed method to link different computational tools such as Ab-initio methods, classical molecular dynamics and monte carlo simulations with the phenomenological Landau-like theory to understand physical problems at longer length and time scales.

[4] Worked to understand microscopic mechanism for superconductivity in Fe-based superconductors using density functional theory calculations.

[5] Worked to understand the effect of chemical disorder on properties of materials; For examples tried to understand using density function theory calculations

(a) How does very small substitution of $NaNbO_3$ change the properties of $CaTiO_3$ using VCA and supercell approximation

(b) How do doping of different cations in CeO_2 enhance its oxygen storage/release properties.

(c) Why bulk modulus of Sn_3N_4 is relatively small compared to Ge_3N_4 and C_3N_4.

[6] Worked on rare-event problems (where waiting time for a process to occur is many order magnitudes larger than its completion time), such as crystallization of supercooled liquids in the bulk as well as in the finite size systems using multiscale methods.

Feb-March 2010 **Visitor, Prof. Karin Rabe, Department of Physics and Astronomy, Rutgers University, NJ, USA**: Worked towards the development of first-principles effective Hamiltonian for multiferroics material $YMnO_3$ to understand temperature dependent study of the sequences of ferroelectric and anti-ferromagnetic phase transitions and other physical properties.

June-Aug 2009 **Summer Intern, General Electric, Bangalore**: Worked on the fist-principles based modeling to increase the mobility of majority charge carriers at the interface of SiC MOSFET gate oxide and oxidation process at the surfaces of alloys.

Experimental

2004-2005 During my M.Sc. project, I used different experimental techniques such as Transmission Electron Microscope (TEM), Scanning Electron Microscope (SEM), X-ray Diffraction (XRD) and UV-visible spectroscopy to study change in the band gap with nanoparticles diameters.

Computational Skills

DFT Packages: Quantum-Espresso, Abinit, VASP, Siesta

MD Packages: FERAM, Gromacs, LAMMPS, Amber and self written MD and MC Codes

Mathematical Softwares: Mathematica, Matlab

Programming Language: Basic, Fortran, C, Pascal, MPI Parallel Programming

Operating System: Linux, Windows, Mac

Visualization Tools: XcrysDen, Jmol, VMD, VESTA

Plotting Tools: Xmgr, Xmgrace, GNU plot

Research Fellowship and Awards

1 Junior Research Fellowship (JRF) and Eligibility for Lectureship in Physical Sciences by Council of Scientific and Industrial Research (CSIR), India in 2005. This is a national level exam for the research fellowship and eligibility for teaching in the Indian universities.

2 Qualified in the Graduate Aptitude Test in Engineering (GATE-2005). This is a national level test for admission into Master of Technology M. Tech. and PhD programs in India.

3 Qualified in the Joint Entrance Screening Test (JEST-2005). This is a national level test for admission into PhD programs in India

4 Best Poster Award (Theory/Experiment) in the Aspen Conference on Advances in Fundamental Physics of Ferroelectrics and Related Materials, Aspen, CO, USA (February, 2010).

5 I2CAM Travel Award for attending the conference on Fundamental Physics of Ferroelectrics and Related Materials, Aspen, CO, USA (2010).

Presentations

Oral

2014 First-Principles Study of Twinning-Associated Boundaries in HCP Metals, **Anil Kumar**, Jian Wang and Carlos Tome, **MRS Spring Meeting**, San Francisco, CA, USA (April 23, 2014)

2013 First-order metal-insulator transitions in vanadates from first principles, **Anil Kumar** and Karin M Rabe, **APS March Meeting**, Baltimore, MD, USA (March 18, 2013)

2012 First-principles study of the structural and magnetic phase transition in $CdCr_2O_4$, **Anil Kumar** and Karin M Rabe, **APS March Meeting**, Boston, MA, USA (March 01, 2012)

2011 Interatomic force constants and effective Hamiltonians for structural phase transitions, **Anil Kumar** and Karin M Rabe, **APS March Meeting**, Dallas, TX, USA (March 23, 2011)

2010 First-principles Determination of Free Energies of Ferroelectric Phase Transitions and Domains in $BaTiO_3$, **Anil Kumar** and Umesh V Waghmare, **APS March Meeting**, Portland, OR, USA (March 18, 2010)

2009 First-principles Study of $FeSe_{1-x}$: An Iron-based Superconductors, **Anil Kumar**, Umesh V Waghmare and A K Sood, **5^{th} JNC Research Conference on Materials**, Alleppey, Kerala, India, (October 04, 2009)

2008 Free Energies of Ferroelectric Phase Transition: A First-principles Molecular Dynamics Study, **Anil Kumar** and Umesh V Waghmare, **Annual JNC In-house Symposium**, JNCASR, Bangalore, India (November 21, 2008)

Poster

2013 Search for first-order metal-insulator transitions in vanadates from first principles, **Anil Kumar** and Karin M Rabe, **Electronic Structure Workshop**, Williamsburg, VA, USA (Jun 12, 2013)

2013 Domain formation and dielectric response in PbTiO3: A first-principles free energy landscape analysis, **Anil Kumar**, Karin M. Rabe and Umesh V. Waghmare, **APS March Meeting**, Baltimore, MD, USA (March 19, 2013)

2011 Efficient construction of effective Hamiltonians for structural phase transitions, **Anil Kumar** and Karin Rabe, **Ferroelectric Conference**, NIST, MD, USA (Jan 30-Feb 2, 2011)

2010 First-principles Analysis of Electron Correlation, Spin Ordering and Phonons in the Normal State of $FeSe_{1-x}$, **Anil Kumar**, Pradeep Kumar, Umesh V Waghmare and A. K. Sood, **APS March Meeting**, Portland, OR, USA (March 16, 2010)

2010 First-principles Determination of Free Energies of Ferroelectric Phase Transitions and Domains in $BaTiO_3$ and $PbTiO_3$, **Anil Kumar** and Umesh V Waghmare, **Conference on Advances in Fundamental Physics of Ferroelectric and Related Materials**, Aspen, CO, USA (February 1-6, 2010)

Workshops

2009 School and Conference on Multiscale Modeling and Simulations of Hard and Soft Materials, JNCASR, Bangalore (December 7-20, 2009)

2008 International Conference on Molecules to Materials: A New Directions and Winter School on New Carbon Materials and Functional Oxides,JNCASR, Bangalore (December 4-13, 2008)

2007 School on Biomolecular Simulations, JNCASR, Bangalore (November 6-16, 2007)

2007 Spring College on Water in Physics, Chemistry and Biology, ICTP, Trieste, Italy (April 10-21, 2007)

2007 School on Understanding Molecular Simulations and Conference on Nucleation, Aggregation, and Growth, JNCASR, Bangalore (January 22-31, 2007)

2006 Winter School on Chemistry of Materials, JNCASR, Bangalore (December 12-19, 2006)

2006 Harvard-JNCASR-NCBS Symposium, NCBS, Bangalore (August 11-13, 2006)

2006 Summer School on Electronic Structure Methods and Applications and Workshops on Computational Material Theory, JNCASR, Bangalore (July 20-30, 2006)

Publications

Preprint

[24] First-principles analysis of structure and energies of Mg/Nb interface, **Anil Kumar**, Jian Wang and Irene Beyerlein (2014 manuscript under preparation)

[23] An unconventional fcc to hcp phase transformation mechanism in hcp metals, Haichen Wu, **Anil Kumar**, Lei Liu, Xiaofang Bi, Carlos N Tome, Jian Wang (2014 manuscript under preparation)

[22] Observation of free volume at twin boundaries in HCP metals from density functional theory calculations, **Anil Kumar**, Jian Wang and Carlos Tome (2014 manuscript under preparation)

[21] Solute selection using density functional theory calculations to minimize $(10\bar{1}2)$ twin boundary energy in Mg and Ti, **Anil Kumar**, Jian Wang and Carlos Tome (2014 manuscript under preparation)

[20] Evidence for an isostructural phase transition within the stability field of the orthorhombic phase of $CaTiO_3$, Saurabh Tripathi, **Anil Kumar**, Masatomo Yashima, U. V. Waghmare, Dhananjai Pandey (2014 manuscript under preparation)

[19] Composition induced phase transitions in lead free and non ferroelectric constituent system $(1-x)$$NaNbO_3$-$x$$CaTiO_3$: Anomalies in the amplitude of phonon modes and evidence for an isostructural morphotropic phase transition, Saurabh Tripathi, **Anil Kumar**, Sanjay Kumar Mishra, P.S.R. Krishna, Umesh Waghmare and Dhananjai Pandey (2014 manuscript under preparation)

[18] Evolution of Oxygen Storage Capacity originating from phase transformation of pyrochlore-$Ce_2Zr_2O_7$ to fluorite-$Ce_2Zr_2O_8$, Asha Gupta, **Anil Kumar**, Umesh Waghmare, and M.S. Hegde (2014 manuscript under preparation)

[17] Metal-insulator transition in Ruddlesden-Popper series of $Sr_{n+1}Co_nO_{3n+1}$, **Anil Kumar** and Karin M. Rabe, (2014 manuscript under preparation)

[16] First-principles search for first order metal-insulator transition in perovskite vanadates, **Anil Kumar**, and K. M. Rabe, (2014 manuscript under preparation)

[15] Efficient construction of first-principles effective Hamiltonians for structural phase transitions, **Anil Kumar**, Qibin Zhou and Karin M. Rabe, (2014 manuscript under preparation)

Published

[14] Domain formation and dielectric response in $PbTiO_3$: A first-principles free-energy landscape analysis, **Anil Kumar**, K. M. Rabe and U. V. Waghmare, Phys. Rev. B 87, 024107 (2013), [**Selected as Editor's suggestion**]

[13] Spin-lattice coupling and phonon dispersion of $CdCr_2O_4$ from first principles, **A. Kumar**, C. J. Fennie and K. M. Rabe, Phys. Rev. B. 86, 184429 (2012)

[12] Structural phase transition below 250 K in superconducting $K_{0.75}Fe_{1.75}Se_2$, A. Ignatov, A. Kumar, P. Lubik, R. H. Yuan, W. T Guo, N. L. Wang, K. Rabe, G. Blumberg, Phys. Rev. B. 86, 134107 (2012), [**Selected as Editor's suggestion**]

[11] Molecular Dynamics Simulation of 90^o Ferroelectric Domains in $PbTiO_3$, Takeshi Nishimatsu, Kenta Aoyagi, Takanori Kiguchi, Toyohiko J. Konno, Yoshiyuki Kawazoe, Hiroshi Funakubo, **Anil Kumar** and Umesh V. Waghmare, J. Phys. Soc. Jpn. 81, 124702 (2012)

[10] Raman evidence for superconducting gap and spin-phonon coupling in superconductor $Ca(Fe_{0.95}Co_{0.05})_2As_2$, Pradeep Kumar, Achintya Bera, D. V. S. Muthu, **Anil Kumar**, U. V. Waghmare, L. Harnagea, C. Hess, S. Wurmehl, S. Singh, B. Büchner and A. K. Sood, J. Phys. Condens Matter, 23, 255403 (2011).

[9] Elastic and structural instability of cubic Sn_3N_4 and C_3N_4 under pressure, Gopal K. Pradhan, **Anil Kumar**, Umesh V. Waghmare, Sudip K. Dev and Chandrabhas Narayan, Phys. Rev. B, 82, 144112 (2010)

[8] First-principles analysis of electron correlation, spin ordering and phonons in the normal state of $FeSe_{1-x}$, **Anil Kumar**, Pradeep Kumar, Umesh Waghmare, Ajay K Sood, J. Phys.: Condens Matter, 22, 385701 (2010)

[7] First-principles free energies and Ginzburg-Landau theory of domains and ferroelectric phase transitions in $BaTiO_3$, **Anil Kumar** and Umesh V. Waghmare, Phys. Rev. B, 82, 054117 (2010)

[6] Temperature-dependent Raman study of a $CeO_{0.9}F_{0.1}FeAs$ Superconductor: crystal field excitations, phonons and their coupling, Pradeep Kumar, **Anil Kumar**, Surajit Saha, D. V. S. Muthu, J. Prakash, U. V. Waghmare, A. K. Ganguli, and A. K. Sood, J. Phys.: Condens. Matter **22**, 255402 (2010)

[5] The effect of $NaNbO_3$ substitution on the quantum paraelectric behavior of $CaTiO_3$, Saurabh Tripathi, **Anil Kumar**, Umesh V. Waghmare, and Dhananjai Pandey, Phys. Rev. B. **81**, 212101 (2010)

[4] First-principles analysis of structural stability in Ce_{1-x} SnO_2, Asha Gupta, **Anil Kumar**, M.S. Hegde, Umesh V. Waghmare, J. Chem. Phys. **132**, 194702 (2010)

[3] Anomalous Raman scattering from phonons and electrons of superconducting $FeSe_{0.82}$, Pradeep Kumar, **Anil Kumar**, Surajit Saha, D. V. S. Muthu, J. Prakash, S. Patnaik, U. V. Waghmare, A. K. Ganguli, and A. K. Sood, Fast Track Solid State Communications **150**, 557 (2010)

[3] Anomalous Raman scattering from phonons and electrons of superconducting $FeSe_{0.82}$, Pradeep Kumar, **Anil Kumar**, Surajit Saha, D. V. S. Muthu, J. Prakash, S. Patnaik, U. V. Waghmare, A. K. Ganguli, and A. K. Sood, Fast Track Solid State Communications **150**, 557 (2010)

[2] Origin of activation of Lattice Oxygen and Synergistic Interaction in Bimetal-Ionic $Cd_{0.89}Fe_{0.1}Pd_{0.01}O_{2-\delta}$ catalyst , Asha Gupta,**Anil Kumar**, Umesh V. Waghmare and M. S. Hegde, Chemistry of Materials, **21**, 4880 (2009)

[1] $Si_xC_{1-x}O_2$ alloys: A possible route to stabilize carbon-based silica-like solids?, A. Aravindh,...**Anil Kumar**,...Shobhana Narashimhan et al, Solid State Commun. **144**, 273 (2007)

Service Contributions

Reviewer

Materials Research Letters, Acta Materialia, Solid State Communication, J. Phys. Chem., Scientific Reports, International Journal of Plasticity etc

Session Chair

MRS Spring symposium: TEM Characterization and Atomic-Level Modeling of Deformation Mechanisms (2014)